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Sensitivity analysis of the energy density in a thermo chemical heat storage device

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Abstract

Numerical simulation is used to present the spatial and temporal evolution of the temperature, the moisture content, the energy density and the instantaneous power in a fixed bed of zeolite beads during water adsorption. The sensitivity of the released energy density to some parameters (reactor geometry, feed relative humidity and temperature, kinetic coefficient, wall heat transfer coefficient, axial mass and thermal dispersion, permeability) is analyzed. To obtain optimal performances from the fixed-bed reactor and to meet the heating needs of a building, balance has to be found between the latter variables since they have an influence on the discharge duration and the power levels obtained.

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Keywords: thermal energy storage; zeolite; heat and mass transfer; sorption; energy density; instantaneous power.

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1. Introduction

The primary role of thermal energy storage systems is to diminish the discrepancy between the availability of resources and their demand [1, 2]. In addition, designing efficient and inexpensive energy storage devices is vital since energy supply will become more and more volatile, as a consequence of the increasing share of renewable energies, which are inherently intermittent, in the energy mix. Furthermore, the usage of a storage system during consumption peaks [3, 4], by punctual discharges, contributes to smoothing the load curve and avoids the usage of the most polluting power plants.

Several international open adsorption seasonal storage projects aiming to show the feasibility and relevance of such systems have emerged in recent years [2, 5, 6, and 7]. The results of these studies show there remain some uncertainties as to how to choose the adequate material and about the power levels reached by the reactor.

The thermal storage system we wish to design, with the sorption couple zeolite/water, uses excess solar heat during the summer (the regeneration phase) and the indoor humid air during winter (the discharging phase). In order to reach the desired performances, heat and mass transfer in the storage device have to be optimized with the following criteria in mind: a high storage energy density, temperature levels in line with those required for space heating and an important power density.

The design and simulation of a sorption heat storage fixed-bed reactor involves the mathematical modeling of the transport and sorption processes occurring in a multi-phase (gaseous, adsorbed and solid states) system. In this work, a pseudo-homogeneous model, which does not explicitly account for the presence of the sorbent beads, has been established in order to simulate the performance of a fixed bed of zeolite beads during the adsorption of water (the discharging phase). While there are correlations available in the literature for the description of some parameters, their influence on the energy density and instantaneous power released has to be checked in order to evaluate the impact of an inadequate estimate of the latter.

Nomenclature

c_v, c_f	water vapour and total concentration	mol/m^3
C_{p_f}, C_{p_b}, C_p^a	fluid, bead and adsorbed phase heat capacity	J/kgK
D_k, D_m, D_b	Knudsen, molecular and bead effective diffusivity	m^2/s
D_z	axial mass dispersion coefficient	m^2/s
h_i, h_e	heat transfer coefficient at the internal and the external wall	W/m^2K
L	length of adsorption column	m
K_z	effective axial thermal conductivity	W/mK
K	permeability	m^2
k_{ldf}	LDF mass transfer coefficients	$1/s, m/s$
M_a	molar mass of adsorbed phase	kg/mol
Nu	Nusselt number	
P	pressure	Pa
Pe	Peclet number	
ΔP	power released	W
$\bar{q}, \tilde{q}$	volume averaged amount adsorbed and spatial mean of $\bar{q}$	mol_{H2O}/kg_{ads}
q_{eq}	equilibrium amount adsorbed	mol_{H2O}/kg_{ads}
$Q_{v_{in}}$	feed volume flow rate	m^3/s
R_b, R_{B_i}, R_{B_e}	bead and adsorption column (internal and external) radius	m
Re, Sc	Reynolds, Schmidt number	
$T_{in}, T, T_{amb}, T_{out}, T_w$	feed, bed, ambient, wall and effluent temperature	K
u_D, u	superficial, interstitial velocity	m/s
$x_{v_{in}}, x_v$	feed and bed water vapour molar fraction	
z	axial distance along the fixed bed	m
ΔE	energy density released	J/m^3

ΔH	heat of adsorption	*J/mol*
ρ_f, ρ_b, ρ_w	fluid, bead and wall density	kg/m^3
$\varepsilon, \varepsilon_b$	fixed-bed and bead porosity	
λ_f, λ_b	fluid and bead thermal conductivity	*W/mK*
Ω	volume	m^3

2. Mathematical modeling

The feed gas, humid air, is supplied to the bed at ambient temperature. The equations which govern heat and mass transfer in porous media are generally obtained by means of scale-changing methods [8]. Such methods allow moving from a microscopic scale, in which the averaging volume is small compared to the pores, to a macroscopic scale, in which the averaging volume is large next to the pores. The actual discontinuous medium is thus converted, under certain closure assumptions, to an equivalent fictitious continuous one.

The hypotheses to which the equations in the model describing the dynamics of the system are subject to are as follows:

(1) The adsorbent beads have identical properties and are uniformly distributed throughout the bed;
(2) The bed porosity is uniform;
(3) The gas phase behaves as an ideal gas mixture of dry air and water vapour;
(4) Thermal equilibrium is assumed between the three phases (solid, gas, and adsorbed);
(5) The flow pattern can be described by an axially dispersed plug flow-model;
(6) Radial gradients in the bed are negligible;
(7) Axial conduction in the wall is negligible.

Considering the above assumptions, the macroscopic equations governing heat and mass transfer in the bed are:

(1) Overall mass balance:

$$\frac{\partial(\varepsilon c_f)}{\partial t} = -\frac{\partial(u_D c_f)}{\partial z} - (1-\varepsilon)\rho_b \frac{\partial \bar{q}}{\partial t} \tag{1}$$

(2) Component (water vapour) mass balance, where, x_v, in eq. (2-b) is the water vapour molar fraction:

$$c_f \frac{\partial(\varepsilon x_v)}{\partial t} = -c_f u_D \frac{\partial x_v}{\partial z} + \frac{\partial}{\partial z}\left(D_z c_f \frac{\partial x_v}{\partial z}\right) - (1-\varepsilon)\rho_b \frac{\partial \bar{q}}{\partial t}(1-x_v) \tag{2-a}$$

$$x_v = \frac{c_v}{c_f} \tag{2-b}$$

The axial dispersion term is expressed as a function of the water vapour molar fraction according to the method of Choong et al. [9].

(3) The energy balance with heat transfer to the wall:

$$\left[\alpha\left(\rho C_p\right)_f + \left(\rho C_p\right)_b^*\right]\frac{\partial T}{\partial t} = -\left(\rho C_p\right)_f u_D \frac{\partial T}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial T}{\partial z}\right) - (-\Delta H)(1-\varepsilon)\rho_b \frac{\partial \bar{q}}{\partial t} - \frac{2h_i}{R_{B_i}}(T - T_w) \tag{3-a}$$

$$\left(\rho C_p\right)_b^* = (1-\varepsilon)\left[\left(\rho C_p\right)_b + \bar{q}\rho_b C_p^a M_a\right] \tag{3-b}$$

$$\alpha = \varepsilon + (1-\varepsilon)\varepsilon_b \tag{3-c}$$

(4) The heat loss through the wall:

$$\left(\rho C_p\right)_w S_w \frac{\partial T_w}{\partial t} = 2\pi R_{B_i} h_i (T - T_w) - 2\pi R_{B_e} h_e (T_w - T_{amb}) \tag{4-a}$$

$$S_w = \pi\left(R_{B_e}^2 - R_{B_i}^2\right) \tag{4-b}$$

Equilibrium isotherm and kinetics of adsorption

The linear driving force (LDF) model [10] is used to predict the adsorption rate:

$$\frac{\partial \bar{q}}{\partial t} = k_{ldf}\left(q_{eq} - \bar{q}\right) \tag{5}$$

The coefficient, k_{ldf}, in eq. (5), is a lumped parameter which takes into account the different mass transfer resistances the water molecules encounter before reaching the adsorption sites.

Although the LDF approximation underestimates the adsorbed quantities at short times, the predictions are quite accurate over sufficiently long time intervals.

In this study, a polynomial interpolation is used to evaluate the adsorption equilibrium of water on the zeolite beads, which is generally considered to be type II according to Brunauer's classification:

$$q_{eq} = q_{max}\left(b_1 + red\left(b_2 + red\left(b_3 + red\left(b_4 + red(b_5 + red * b_6)\right)\right)\right)\right) \tag{6-a}$$

$$red = c_v/c_{max} \tag{6-b}$$

Where:

$$c_{max} = a_2T^2 + a_1T + a_0 \tag{6-c}$$

The coefficients b_i and a_i are obtained via polynomial interpolation from the experimental data of Ahn and Lee [11].

Mass and thermal axial dispersion

The correlation of Wakao and Funazkri [12] is used to estimate mass axial dispersion:

$$D_z = 2uR_b\left(\frac{20}{ReSc} + 0.5\right) \tag{7}$$

As for the effective axial thermal conductivity, it can be given by [13]:

$$K_z \left(\rho C_p\right)_f \Big/ \lambda_f = \lambda_{eff} \Big/ \lambda_f + 0.8\, Pe \tag{8-a}$$

Where:

$$\lambda_{eff} = \lambda_b^{(1-\varepsilon)}\lambda_f^{\varepsilon} \tag{8-b}$$

$$Pe = u_D 2R_b\left(\rho C_p\right)_f \Big/ \lambda_f \tag{8-c}$$

Velocity

The velocity is described by Darcy's law:

$$u_D = -\frac{K}{\mu}\frac{\partial P}{\partial z} \tag{9-a}$$

Where K is estimated from Karman-Kozeny's equation [8], for spherical beads:

$$K = \frac{\varepsilon^3}{150(1-\varepsilon^2)}(2R_b)^2 \tag{9-b}$$

Wall heat transfer

The correlation Yagi and Wakao [14] is used to evaluate the heat transfer coefficient at the inner wall of the column:

$$Nu_w = 0.17Re^{0.79} \tag{10}$$

Initial and boundary conditions

During the discharging phase, the initial conditions are as follows:

$$\bar{q}(0,z) = 0, x_v(0,z) = 0,\ C_f(0,z) = C_0,\ T(0,z) = T_{amb} \tag{11}$$

As for the boundary conditions:

Table 1: Boundary conditions

	$u_D C_f$	x_v	T	
$z = 0$	$u_D C_f = {Q_{v_{in}}}/{S_B C_{f_{in}}}$	$D_z \frac{\partial x_v}{\partial z} = u_D(x_v - x_{v_{in}})$	$\lambda_z \frac{\partial T}{\partial z} = u_D(\rho C_p)_f (T - T_{in})$	(12-a)
$z = L$		$\frac{\partial x_v}{\partial z} = 0$	$\frac{\partial T}{\partial z} = 0$	(12-b)

2.1. Physical quantities of interest

After outlining the hypotheses to which the equations in the pseudo-homogeneous model describing the dynamics of the system are subject to, the amount of energy released, which depends on the moisture content of the bed, is estimated as follows [7]:

$$\Delta E(t) = -(1-\varepsilon)\rho_b |\Delta H| [\tilde{q}(t) - \tilde{q}(t_0)] \tag{13-a}$$

Where:

$$\tilde{q}(t) = \frac{\int_\Omega \bar{q}(t) d\Omega}{\int_\Omega d\Omega} \tag{13-b}$$

As for the instantaneous power released by the bed, it is given by:

$$\Delta P(t) = Q_{v_{in}} (\rho C_p)_{f_{in}} \left(T_{out}(t) - T_{in}(t)\right) \tag{14}$$

2.2. Numerical simulation

First order upwind and second order central finite difference schemes are used to approximate the first and second order spatial derivatives. The set of the partial differential equations (PDEs) describing the dynamics of the system are solved using the DASSL algorithm in Dymola©.
The CPU time for solving the above is approximately 0.2 seconds on a computer (PC, 3.0 GHz).

3. Results and discussion

3.1. Validation of the numerical simulation

The numerical simulation is validated with experimental data [11, 15, 16] of a TSA process. The adsorption bed has an inner diameter of 3 cm; the wall thickness is of 0.23 cm and the bed height is of 30 cm. The adsorption conditions are as follows: the ambient temperature is equal to about 24°C with a relative humidity of around 55%; the feed flow rate is equal to 9l/min.

The calculated temperature and "dimensionless" water vapour molar fraction as well as the experimental values are plotted in figure 1. The results are quite satisfactory, especially when it comes to the description of the temporal evolution of the water vapour molar fraction. As far as temperature is concerned, the general trends are good enough.

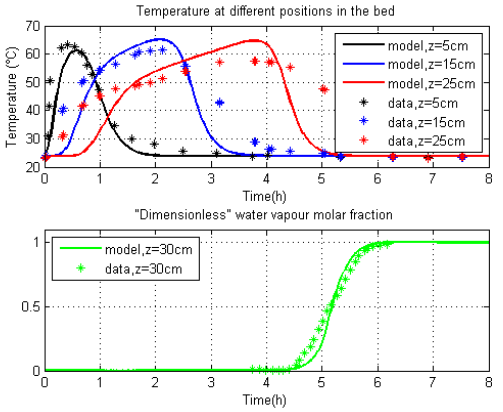

Figure 1: Temperature at different positions in the bed and "dimensionless" water vapour molar fraction

3.2. Preliminary sensitivity studies

The aim is to assess the sensitivity of the energy density and the instantaneous power released during the discharging phase to variations of the model parameters and variations of model assumptions. Indeed, the proper evaluation of parameters such as k_{ldf}, h_i, D_z and K_z is a tricky issue, despite the presence of different correlations in the literature. It is thus essential to evaluate to which extent an incorrect estimate of the latter affects the outputs of interest. The results reported below represent the preliminary stage of this sensitivity analysis since only first order interactions are studied.

Effect of the LDF parameter

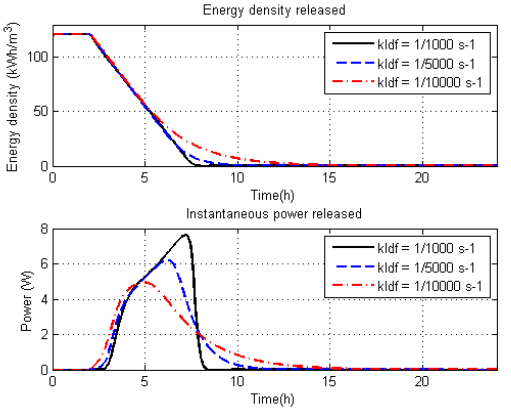

Figure 2: Influence of the LDF parameter on the energy density and instantaneous power released

As can be seen in figure 2 above, an increase of the adsorption coefficient results in a reduction of the discharge duration. Indeed, the energy density in the bed decreases at a slower rate when the LDF parameter is reduced. A higher constant of adsorption indicates that the water molecules take less time to overcome the mass transfer resistances they encounter. Therefore, higher values of the LDF parameter lead to smaller discharge durations. Moreover, the instantaneous power released is affected to a significant degree by a change in this parameter. A proper estimation of the LDF parameter is thus crucial for a good evaluation of the performances of the bed.

Effect of wall heat transfer coefficient

The wall heat transfer coefficient mainly influences the instantaneous power as can be seen in figure 3. For low

values of this parameter the instantaneous power varies considerably. This result was expected since the wall heat transfer coefficient is a lumped parameter representing the radial effects as far as the temperature is concerned.

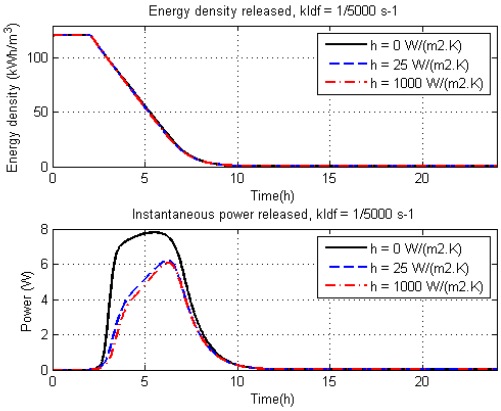

Figure 3: Influence of the wall heat transfer coefficient on the energy density and instantaneous power released

Effect of the mass dispersion coefficient and the effective axial thermal conductivity

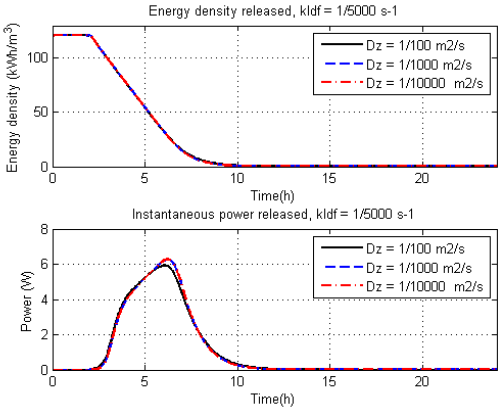

Figure 4: Influence of the masse dispersion on the energy density and instantaneous power released

As for the mass dispersion coefficient and the effective axial thermal conductivity, they seem to have only a slight influence on the outputs of interest as shown in figures 4 and 5.

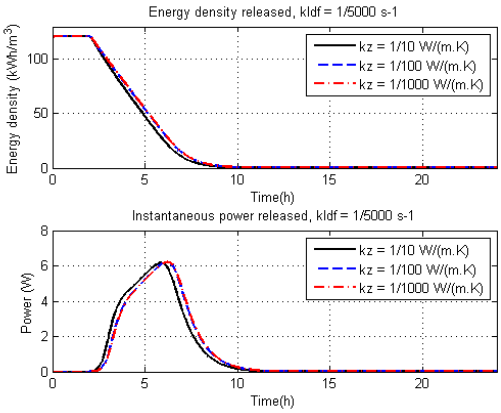

Figure 5: Influence of the effective axial thermal conductivity on the energy density and instantaneous power released

4. Conclusions

A pseudo-homogeneous model describing heat and mass transfer during adsorption of water vapour in a fixed bed packed with zeolite beads was established and solved with finite difference schemes.
The calculated temperature evolves correctly when compared to experimental results.
However, there remain some differences which could be due to:

- the thermal equilibrium assumption;
- the LDF assumption: the LDF the coefficient is assumed to be constant for the time being although it varies with the temperature and the pressure;
- the 1D assumption : the radial effects are lumped into the wall heat transfer coefficient. However, for low Reynolds numbers, which is likely to be the configuration of our study, correctly taking into account wall heat transfer is a tricky issue;

The preliminary results of the sensitivity study show that the LDF parameter and the wall heat transfer coefficient have a significant effect on the instantaneous power released in particular. A proper estimate of the latter is important for the correct evaluation of the energy density and the power in the bed.

Further work will be to carry on with the sensitivity analysis during an entire cycle (discharging and charging phases), with particular attention to the coupled interactions of the different parameters studied here and outputs of interest (released or stored).

Acknowledgements

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